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Study of the effect of magnetic field on the impurity bound polaronic energy levels in a parabolic quantum dot**

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Abstract : The problem of interface optical polaron, bound to an impurity atom in a parabolic quantum dot near the semiconductor heterostructure has been investigated in the framework of canonical transformation method. An external magnetic field is applied in the growing direction of the quantum dot heterostructure (along the *z*-direction). A calculation has been proposed to study the dependence of the ground state energy on the magnetic field and the thickness of the well. The binding energy and hence the quantum confinement increases with the increasing magnetic field. The effect of the thickness on the induced potential and hence on the ground state energy has also been studied.

Keywords : Polaron, semiconductor heterostructure, magnetic field, canonical transformation method.

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1 Introduction

When an electron (externally injected) moves in a polar medium it causes a distortion of the lattice establishing a polarization field which acts back on the electron whose properties are then modified (*i.e.*, the electron digs its own hole). This single electron with the surrounding lattice distortion (the electron with the accumulated virtual phonons) is called a polaron [1,2].

In the recent years, there have been several investigations of polaron effects in polar semiconductor heterostructures such as dielectric slabs, heterojunctions, quantum wires, quantum boxes, quantum dots and quantum well structures [3]. Some usual quantum wells such as GaAs/$Al_xGa_{1-x}As$ quantum well is composed of polar compounds in which the interaction of an electron with optical phonon is an important mechanism that needs to be studied in detail. The polaron effect can strongly influence the optical and transport properties of the heterostructures. Hence the polaron has been a major topic of great interest since a long time. Now a days the interest in the nano-structures with confinement of electrons [4] in all directions (called quantum dots) becomes much important due to the fact that the quantum dot structures have much useful applications in the micro electronic device technology because of their design flexibility. Several authors have studied the confinement of the bulk optical polaron in two dimensional quantum structure [5–7].

In this communication, we study the effect of the interaction of the electron and longitudinal optical phonon in two dimensional semiconductor quantum dot. The purpose of this investigation is to present a detailed study of quantum dot in which magnetic field and impurity binding potential are fully taken into account.

In our model, we have considered that the interface electron is initially bound to a Coulomb type impurity atom near a semiconductor heterojunction in a parabolic confined quantum dot of finite thickness. An external magnetic field is applied in the growing direction of the quantum

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heterostructure (along z-direction). Here as a first approximation we have neglected the effect of the interaction of electron with bulk optical phonon as this effect will be reduced near the heterojunction. We propose a canonical transformation method [8] to study the dependence of the ground state energy, wave function and induced potential on the magnetic field and the thickness of the well.

2. Theory

The model considered is as follows. A quantum dot (of frequency w_0) is confined by a square well in the z-direction and a harmonic potential in the xy plane. The impurity is situated at the origin and a magnetic field is applied along the z-direction. So the Hamiltonian for the interface polaron (assuming that the interaction of the interface electron with the bulk phonons can be neglected) in the dot can be written as [9]

$$H' = \left\{\frac{1}{2m}\left(\underline{p} - \frac{e\underline{A}}{e}\right)^2 - \frac{e^2}{\varepsilon_\infty r'} + \frac{1}{2}m.\omega_0^2\rho'^2 + v(z')\right\}$$

$$+ \left\{\sum_{\underline{q}'} \hbar\omega_s b_{\underline{q}'}^{+} b_{\underline{q}'}\right\}$$

$$+ \sum_{\underline{q}'}\left\{\xi_{\underline{q}'} e^{-q'|z'|} e^{-i\underline{q}'\cdot\underline{\rho}'} b_{\underline{q}'}^{+} + h.c.\right\}$$

$$= h_e + h_p + h_{ep}, \tag{1}$$

where $\xi_{q'} = \frac{i}{\sqrt{q's'}}\hbar\omega_s \; 2\pi\alpha_s\left(\frac{\hbar}{2m\omega_s}\right)^{1/2}$

$$\alpha_s = e^2(E_s - E_\infty)\left(\frac{m}{2\hbar^3\omega_s}\right)^{1/2}$$

$$E_s = \frac{\varepsilon_s - 1}{\varepsilon_s + 1};\; E_\infty = \frac{\varepsilon_\infty - 1}{\varepsilon_\infty + 1}$$

and s' is the area of the interface, ε_0 and ε_s being the static and high-frequency dielectric constant respectively. In the phonon Hamiltonian h_p, w_s is the dispersionless phonon frequency. With the constant magnetic filed B chosen in the z'-direction, the electronic Hamiltonian h_e in cylindrical co-ordinate (x', y, z') is given by

$$h_e = -\frac{\hbar^2\nabla'^2}{2m} + \frac{m}{8}\left(\frac{eB}{mc}\right)^2\rho'^2 - i\hbar\left(\frac{eB}{mc}\right)\frac{\partial}{\partial\delta} - \frac{e^2}{\varepsilon_\infty r}$$

$$+ \frac{1}{2}m\omega_0^2\rho'^2 + v(z'), \tag{2}$$

where $\nabla'^2 = \frac{1}{\rho'}\frac{\partial}{\partial\rho'}\left(\rho'\frac{\partial}{\partial\rho'}\right) + \frac{1}{\rho'^2}\frac{\partial^2}{\partial\phi^2} + \frac{\partial^2}{\partial z'^2}$,

$$\rho'^2 = x'^2 + y'^2,$$

$$A = (A_\rho, A_\phi, A_z) = \left(0, \frac{1}{2}B\rho', 0\right),$$

$$r' = (\rho', \phi, z'),$$

$$v(z') = v_0 \quad -\infty < z' \le 0,$$

$$= 0 \quad 0 < z' < \infty. \tag{3}$$

Taking the unit of length as $a^{-1} = \left(\frac{eB}{2c\hbar}\right)^{-1/2}$ and unit of energy as $\varepsilon_a = \hbar^2a^2/2m = \hbar\omega_s\Lambda^2/4$, $\Lambda^2 = eB/m\omega_s c = \omega_c/\omega_s$ (where w_c is the cyclotron frequency), the Hamiltonian is written in a convenient dimensionless form

$$H = H'/\varepsilon_a = \left\{-\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{1}{\rho^2}\frac{\partial}{\partial\phi^2} - \frac{\partial^2}{\partial z^2} - 2t\frac{\partial}{\partial\phi}\right.$$

$$\left. - \frac{\beta}{2\Lambda}\frac{1}{\rho} + (1 + C^2)\rho^2 + \sum_q \frac{4}{\Lambda^2}b_q + b_q\right.$$

$$\left. + \sum\left\{\xi_q e^{-q|z|} e^{-iq\cdot\rho} + h.c.\right\}\right., \tag{4}$$

where $\xi_q = 4i\left|\frac{\pi\alpha_s}{q}\right|\frac{1}{\Lambda^{3/2}}$,

$$C = \frac{2T}{\Lambda};\; T = \frac{\omega_0}{\omega_c}.$$

This Hamiltonian in eq. (4) is now partially decoupled by a canonical transformation in the usual way [8]

$$H \to H^{(1)} = e^{-U}He^{U} = h_e^{(1)} + h_p + h_{ep}^{(1)},$$

where $U = \sum_{\underline{q}}\left\{\left(\frac{\Lambda^2}{4}\bar{\xi}_q\right)b_q - h.c.\right\}$

and $\bar{\xi}_q = \left\langle\phi_0^{(0)}\middle|\xi_q e^{-q|z|}e^{i\underline{q}\cdot\underline{\rho}}\middle|\phi_0^{(0)}\right\rangle$.

The averaging function is chosen $\left|\phi_0^{(0)}\right\rangle$ which is known from $h_e\left|\phi^{(0)}\right\rangle = \varepsilon^{(0)}\left|\phi^{(0)}\right\rangle$ for the ground state and hence the electron phonon interaction term is modified as

$$h_e^{(1)} = h_e - \sum_{\underline{q}}\left(\frac{\Lambda^2}{4}\overline{\xi_q}\xi_q e^{-q|z|}e^{i\underline{q}\cdot\underline{\rho}} + h.c.\right) + k^{(1)},$$

where $k^{(1)} = \sum_q \frac{\Lambda^2}{4}\left|\left\langle\phi_0^{(0)}\middle|\xi_q e^{-q|z|}e^{i\underline{q}\cdot\underline{\rho}}\middle|\phi_0^{(0)}\right\rangle\right|^2$. (5)

The phonon induced attractive potential is given by

$$V_{in}(\rho,z)=\sum\frac{\Lambda^2}{4}\left\{\xi_q e^{-q|z|}e^{iq\cdot\rho}\bar{\xi}_q+h.c.\right\}$$

$$=\frac{4\alpha_s}{\Lambda}\iint\frac{\phi_0^{(0)}\left|^2\right.dzd\rho'}{\left[(z+z')^2+(\rho-\rho')^2\right]^{1/2}} \quad (6)$$

By applying mean value theorem within a small thickness perpendicular to the intereface $0 < z_0 < d$ and performing $\phi(z')$ integration, the induced potential V_{in} for the ground state becomes

$$V_{in}=4\alpha_s\int\frac{\phi^{(0)}(\rho')\Big|^2 d\rho'}{\left[(z+z_0)^2+(\rho-\rho')^2\right]^{1/2}}. \quad (7)$$

Now for the ground state we choose

$$\phi_0^{(0)}(\rho)\to\phi_0^{(0)}(\rho)=\frac{\beta}{\sqrt{2\pi\Lambda}}e^{-(\beta/2\Lambda)\rho}.$$

The new electronic Hamiltonian $h_e^{(1)}$ becomes finally

$$h_e^{(1)}=\left\{-\nabla_\rho^2+(1+C^2)\rho^2+\frac{\beta}{2\Lambda}\frac{1}{\rho}-V_{in}(\rho,z)\right\}$$

$$+\left\{-\nabla_z^2+v(z)\right\}+\left(\frac{\beta}{2\Lambda\rho}-\frac{\beta}{2\Lambda}\frac{1}{r}\right)$$

$$=h_e^{(1)}(\rho)+h_e^{(1)}(z)+h_{pert}. \quad (8)$$

The solution to this Hamiltonian $h_e^{(1)}$ cannot be obtained simply in a separable form due to the induced potential $V(\rho, z)$. But to a good first approximation, the z-dependence of $V(\rho, z)$ may be ignored by noting that $V(\rho, z)$ is very much likely to be at most weakly dependent on z as for a Coulomb attraction the electron stays close to the surface. Therefore, $V(\rho, z)$ may be replaced in good approximation by $V(\rho, \eta)$ where η is a small constant parameter which replaces $z + z_0$. Neglecting h_{pert} term for the above reason, one obtain the Hamiltonian in a separable form

$$h_e^{(1)}=\left\{-\nabla_\rho^2-\frac{\beta}{2\Lambda}\frac{1}{\rho}+(1+C^2)\rho^2-V_{in}(\rho,\eta)\right\}$$

$$-\frac{\partial^2}{\partial z^2}+v(z)$$

$$=h_e^{(1)}(\rho)+h_e^{(1)}(z). \quad (9)$$

This equation is solved by

$$h_e^{(1)}\Psi_e^{(1)}=\varepsilon_1^{(1)}\Psi_e^{(1)},$$

where $\Psi_e^{(1)}=\phi^{(1)}(\rho)\Psi(z)$

and $$h_e^{(1)}(z)\Psi(z)=\varepsilon_1^{(1)}\Psi(z) \quad (10)$$

$$h_e^{(1)}(\rho)\phi^{(1)}(\rho)=\varepsilon_2^{(1)}\phi^{(1)}(\rho). \quad (11)$$

3. Results and discussion

To find the total energy and wave function we have to solve eqs. (10) and (11), and the total energy will be obtained as $\varepsilon^{(1)}=\varepsilon_1^{(1)}+\varepsilon_2^{(1)}$. As an illustration, we have calculated the binding energy $\varepsilon_2^{(1)}$ of an impurity atom with the electron-phonon interaction in a realistic sample GaAs/$Ga_xAl_{1-x}As$. In the canonically transformed hamiltonian, the electronic part of the hamiltonian ($h_e^{(1)}$) gets an extra attractive potential term V_{in} due to the electron-phonon interaction which becomes more and more attractive if α_s, β increase and T decreases. In Figure 1, the η dependence of V_{in} has been shown for two different values of ρ. The dependence of V_{in} on ρ is very weak except near the surface. In Figure 2, curves (B) and (D) for $T = 1.0$ ($\omega_0 = \omega_c$) with $\Lambda = 1.0$ ($\omega_s = \omega_c$) and $\Lambda = 0.5$ ($\omega_c = 0.5\omega_s$)

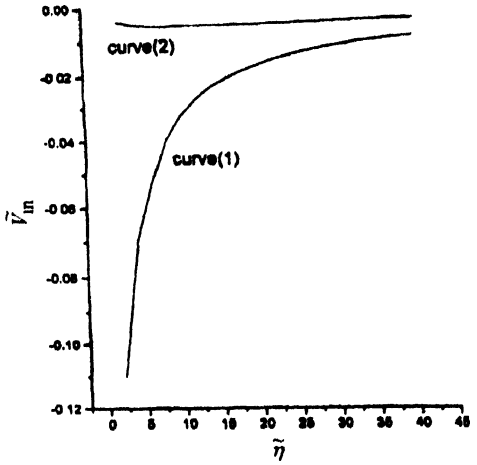

Figure 1. The induced potential $\tilde{V}_{in}(=V_{in}(\rho,\eta)\Lambda^2/4)$ as a function of $\tilde{\eta}(=2\eta/\Lambda)$ in Fröhlich unit (energy unit $\hbar\omega_s$, length unit $\sqrt{\hbar/2m\omega_s}$) for a fixed value of $\alpha = 0.296$, $\beta = 1.0$, $\Lambda = 1.0$, $T = 1.0$. Curve (1) for $\tilde{\rho}(=2\rho/\Lambda) = 0.002$ and curve (2) for $\tilde{\rho} = 1.004$.

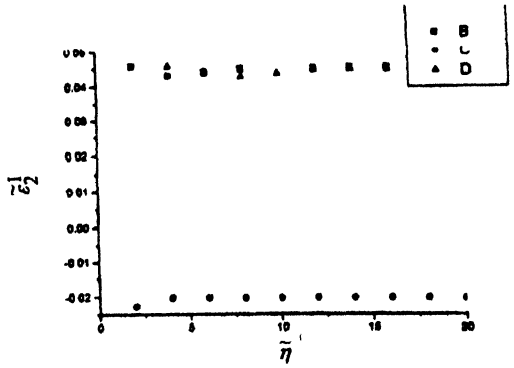

Figure 2. $\tilde{\varepsilon}_2^{(1)}(=\varepsilon_2^{(1)}\Lambda^2/4)$ the interface polaron ground state energy as a function of $\tilde{\eta}$ in Fröhlich unit. Curves (B) and (D) for $T = 1.0$, $\beta = 1.0$, $\alpha = 0.296$ and with $\Lambda = 1.0$ and $\Lambda = 0.5$ respectively and curve (C) for $T = 0.1$, $\beta = 1.0$, $\alpha = 0.296$ and $\Lambda = 1.0$.

respectively for a fixed value of b and a. Curve (B) and Curve (D) has a minimum near $\tilde{\eta} \approx 4.0$ and $\tilde{\eta} \approx 8.0$ respectively. The dependence of $\tilde{\varepsilon}_2^{(1)}$ on the applied magnetic field L can be studied from curves (B) and (D). The binding energy increases generally with increasing field. This is not surprising because the magnetic field not only adds extra binding to the orbiting electron it also enhances the electron-phonon coupling. The minima of (B) and (D) indicate that the polaron gets localized more and more near the surface as the magnetic field increases.

The term h_{pert} in $h_e^{(1)}$ can be looked at in first order Rayleigh-Schrödinger Perturbation Theory (RSPT) with the calculated basis $\varphi_0^{(1)}$. Since we are only interested here to study the energy values of an electron which lies close to the heterojunction, we should choose h small. For such h, the perturbation correction from h_{pert} will be very small.

The values of $\epsilon^{(1)}$ has not been shown here explicity as we have not considered the effect of electron-phonon interaction in eq. (10) as a first step of our calculation.

4. Conclusions

In conclusion it should be stated that the motivation for the present problem is to study the quantum confinement of a polaron near the interface of a heterojunction. So this work may be regarded as the first step of forming the basis function of the interface polaron. Detailed study of this problem is still in progress and will be reported in due course.

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